

Bosons in optical lattices - from the Mott transition to the Tonks-Girardeau gas

S. Wessel^(1,2), F. Alet^(2,3,4), S. Trebst^(2,3), D. Leumann⁽²⁾, M. Troyer^(2,3), G. George Batrouni⁽⁵⁾

⁽¹⁾*Institut für Theoretische Physik III, Universität Stuttgart, 70550 Stuttgart, Germany*

⁽²⁾*Theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland*

⁽³⁾*Computational Laboratory, ETH Zürich, CH-8092 Zürich, Switzerland*

⁽⁴⁾*Service de Physique Théorique, CEA Saclay, 91191 Gif sur Yvette, France*

⁽⁵⁾*Institut Non-Linéaire de Nice, Université de Nice-Sophia Antipolis, 1361 route des Lucioles, 06560 Valbonne, France*

We present results from quantum Monte Carlo simulations of trapped bosons in optical lattices, focusing on the crossover from a gas of softcore bosons to a Tonks-Girardeau gas in a one-dimensional optical lattice. We find that depending on the quantity being measured, the behavior found in the Tonks-Girardeau regime is observed already at relatively small values of the interaction strength. A finite critical value for entering the Tonks-Girardeau regime does not exist. Furthermore, we discuss the computational efficiency of two quantum Monte Carlo methods to simulate large scale trapped bosonic systems: directed loops in stochastic series expansions and the worm algorithm.

KEYWORDS: boson Hubbard model, quantum Monte Carlo, cold atoms, optical lattice, hard-core bosons, Tonks-Girardeau gas

1. Introduction

Interest in the properties, phase transitions and various phases of strongly correlated systems in reduced dimensionality has a very long history in condensed matter physics. The experimental realization of Bose-Einstein condensates (BEC) in traps¹ offered the possibility of studying such phenomena in precisely engineered systems. This goal was eventually achieved by placing the condensates on optical lattices^{2,3} which has the effect of packing the bosonic atoms in close proximity to one another and even producing multiple occupancy of lattice sites. Consequently, strongly correlated systems are produced on such optical lattices which have the advantage of being defect free. However, the lattices are immersed in the confining trap and are consequently not translationally invariant. This makes delicate the task of applying results known in condensed matter physics for translationally invariant systems to BEC on optical lattices. The rush to do this has led to some misunderstandings especially concerning “quantum phase transitions” on the optical lattice.

Our goal here is to use quantum Monte Carlo (QMC) methods, such as the stochastic series expansion (SSE) and the worm algorithm, to study in some detail the properties of BEC on optical lattices and elucidate the nature of the observed “transition”.

The paper is organized as follows. In section 2, we introduce the bosonic Hubbard model used for the description of a cold atomic Bose gas trapped on optical lattices and discuss and compare the techniques to simulate it. We then review the results presented in Ref. 4 in section 3, focusing on observables particularly suited for the detection of local “phases” or structures and the absence of quantum criticality in these inhomogeneous systems. In section 4, new results on the transition to a Tonks-Girardeau gas regime for bosonic systems in one-dimension are presented.

2. Quantum Monte Carlo simulations

2.1 Model

We consider the following Bose Hubbard Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + h.c.) \quad (1)$$

$$+ \frac{U}{2} \sum_i n_i(n_i - 1) + V \sum_i r_i^2 n_i - \mu \sum_i n_i,$$

as a good description of the low energy physics of cold confined bosonic gases.⁵ Here t is the nearest neighbor hopping, U the onsite repulsion between the softcore bosons, μ the chemical potential and V the curvature of the parabolic confining potential imposed by the trap. We use standard notations for the bosonic operators. We furthermore define $\mu_i^{\text{eff}} = \mu - V r_i^2$, which is the local effective chemical potential experienced by a boson at site i .

2.2 Quantum Monte Carlo

The Hamiltonian (1) is particularly well suited for simulations using QMC techniques. Indeed and to our best knowledge, such techniques are the only ones able to simulate efficiently the Hamiltonian (1) for the following reasons :

- They work in *any dimension* (unlike the density matrix renormalization group (DMRG) which is restricted to one-dimensional systems).
- They can be used to obtain both finite *and* zero temperature properties.
- They allow the simulation of *non homogeneous* trapping potentials (unlike series expansion).
- *Large system sizes* can be reached (unlike using exact diagonalization).
- They perform an *exact treatment of all terms* in the Hamiltonian (1) (unlike most analytic approaches).

2.3 Efficiency of non-local quantum Monte Carlo methods

We used the most recent world-line QMC algorithms, the SSE algorithm⁶ with directed loops^{7,8} and the worm algorithm⁹ to perform the simulations based on the open source implementations of the ALPS project.¹⁰

The SSE representation⁶ starts from a Taylor expansion of the partition function in orders of the inverse temperature β :

$$\begin{aligned} Z &= \text{Tr} \exp(-\beta H) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \text{Tr}(-H)^n \\ &= \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{\{i_1, \dots, i_n\}} \langle i_1 | -H | i_2 \rangle \cdots \langle i_n | -H | i_1 \rangle. \end{aligned} \quad (2)$$

This representation of the partition function does not suffer from errors introduced by time discretization and the sampling algorithm can be combined with non-local updates such as directed loops.^{7,8} However, the SSE representation of the partition function corresponds to a perturbation expansion in both, diagonal and off-diagonal, terms of the Hamiltonian. For the simulation of trapped bosonic systems we are naturally interested in the limit where the diagonal matrix elements (e.g. the trapping potential) are large. In this limit the SSE sampling can face a considerable slowdown as the probability of exchanging off-diagonal and diagonal bond terms in the Hamiltonian is suppressed. On the contrary, the worm algorithm⁹ samples world lines in the path integral representation of the partition function which treats only the off-diagonal terms in the Hamiltonian as a perturbation

$$Z = \text{Tr} (e^{-\beta H}) = \text{Tr} \left(e^{-\beta H_0} T e^{-\int_0^\beta d\tau V(\tau)} \right). \quad (3)$$

The directed loop and worm algorithms both work in an extended configuration space, which in addition to closed world line configurations, allows for the presence of an open world line fragment, the “worm” or “directed loop”, which is formally introduced by adding a source term to the Hamiltonian

$$H_{\text{worm}} = H - \eta \sum_i (b_i^+ + b_i). \quad (4)$$

This source term allows the world lines to be broken with a matrix element proportional to η . To generate new closed loop configurations in the sampling process, a worm is created and a random sequence of local updates of the worm is performed where each move fulfills detailed balance. Nevertheless, this update procedure can perform non-local changes of the world line configurations as the worm can wind around the lattice in the temporal or spatial direction and thereby change the particle or winding number respectively.

To discuss the computational performance of the two QMC algorithms in simulating confined ultra-cold bosonic atoms in two dimensions we compare the statistical error obtained for the Monte Carlo estimates of observables from simulation runs with a fixed amount

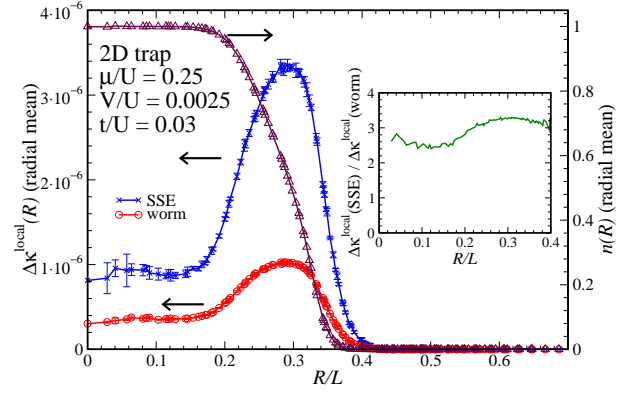


Fig. 1. Comparison of the statistical error $\Delta\kappa^{\text{local}}$ of the local compressibility κ^{local} of a 2D trap with 35×35 sites obtained from simulation runs with fixed CPU-time for stochastic series expansion (SSE) quantum Monte Carlo and the worm algorithm. The error bars are obtained by averaging over estimates with identical radial distance. The inset shows the ratio of statistical errors $\Delta\kappa^{\text{local}}(\text{SSE})/\Delta\kappa^{\text{local}}(\text{worm})$ for the two algorithms using the open-source implementations of the ALPS project.¹⁰

of CPU time (typically around 100 CPU hours on an Opteron 1.8 GHz processor).

While in the homogenous Bose-Hubbard Hamiltonian without confining potential the SSE representation is found to perform better, except from the extreme soft-core case,¹¹ the situation is different when simulating harmonic traps. In Fig. 1 results of our simulations are shown for a two-dimensional system with 35×35 sites and trap parameters which allow for a Mott plateau with integer density ($\langle n_i \rangle = 1$) in the center of the trap ($R/L \lesssim 0.2$). Before discussing the physics of this system in the next sections we first consider the statistical error of the local compressibility κ^{local} (defined by Eq. (5), below), which is shown in Fig. 1 as a function of the distance from the trap center. While for both algorithms the statistical error is largest for the superfluid ring surrounding the central Mott plateau ($0.2 \lesssim R \lesssim 0.4$), the worm algorithm yields a statistical error which is a factor of 3 smaller than the one obtained for the SSE estimate with the same amount of CPU-time. The superior performance of the worm algorithm is a consequence of the small ratio of off-diagonal to diagonal matrix elements for the used value of $t/U = 0.03$ in the simulated Bose-Hubbard Hamiltonian. Further reducing this ratio, e.g. to study trapped bosonic systems which exhibit more than one Mott plateau, will result in an even larger speedup of the worm algorithm.

Fig. 2 shows the ratio of statistical errors of QMC estimates for three different observables obtained using the SSE and worm algorithm. The statistical errors are shown versus the number of lattice sites. For the particle number n and the compressibility κ^{local} (c.f. Eq. (5)) spatial averages are shown. There appears to be a constant improvement of the worm code over the SSE algorithm, independent of the system size, implying that both algorithms exhibit the same scaling in system size. From our simulations we conclude that the worm algorithm is the superior QMC technique to simulate trapped ultra-cold

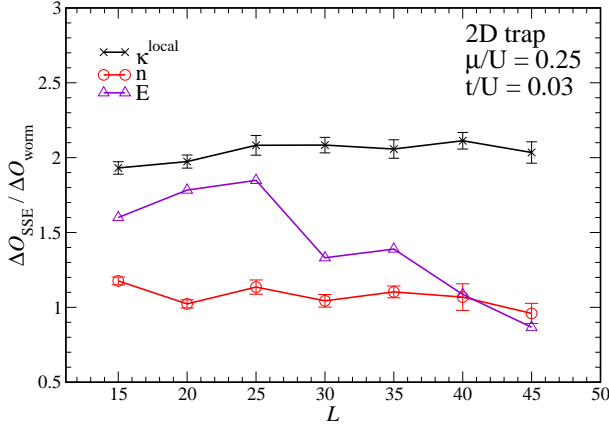


Fig. 2. Scaling of the speedup of the worm algorithm compared to the SSE algorithm versus system size for the same trap parameters as in Fig. 1. Shown are results for the spatially averaged local density n and compressibility κ^{local} as well as the energy E . For all simulations the open-source implementations of the ALPS project¹⁰ were used.

bosonic systems.

3. Simulations of trapped bosonic atoms

3.1 Coexistence of phases and identification of local structures

As shown in various studies (see for example Refs. 2,3 for experimental and Refs. 5,12 for theoretical/numerical investigations), the inhomogeneity in the system due to the trapping potential induces a co-existence of superfluid and Mott insulator-like regions. This can be understood on qualitative grounds by looking at density profiles: a region of space with constant integer density of particles is interpreted as a Mott insulating region (a Mott plateau), while non-integer densities correspond to superfluid regions. To distinguish the state near a given site more precisely, we proposed a more quantitative probe, which will be reviewed here.⁴

For the homogeneous case, the Mott insulating phase has a vanishing compressibility κ .¹³ One way of locally characterizing a region of space in the inhomogeneous system is to study the local compressibility at a given lattice-site i :

$$\kappa_i^{\text{local}} = \left\langle \frac{\partial n}{\partial \mu_i^{\text{eff}}} \right\rangle = \beta (\langle n_i n \rangle - \langle n_i \rangle \langle n \rangle), \quad (5)$$

which expresses the *total* density response of the system to a *local* change of the chemical potential at site i . This local compressibility directly corresponds to the total compressibility κ in the homogeneous case, and serves to distinguish the local states in the inhomogeneous system: κ_i^{local} is zero in a Mott insulating region while it remains finite superfluid region. In Fig. 3, we show the spatial distribution of κ_i^{local} in a two dimensional trapped system. Regions of space with vanishing κ_i^{local} are clearly identified and correspond to Mott insulating regions in the sample.

For the Hamiltonian in Eq. (1), the kinetic term t , the repulsion U and the trap curvature V are tunable parameters in the experiments,^{2,3,19–22} and a “quantum

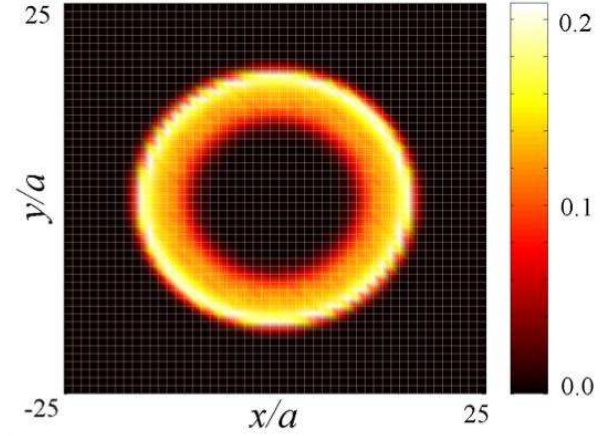


Fig. 3. Spatial dependence of the local compressibility κ^{local} , of bosons in a two dimensional parabolic trap with curvature $V/U = 0.002$, for $\mu/U = 0.37$ and $U/t = 25$. A superfluid ring surrounding a $n = 1$ central Mott plateau is clearly resolved.

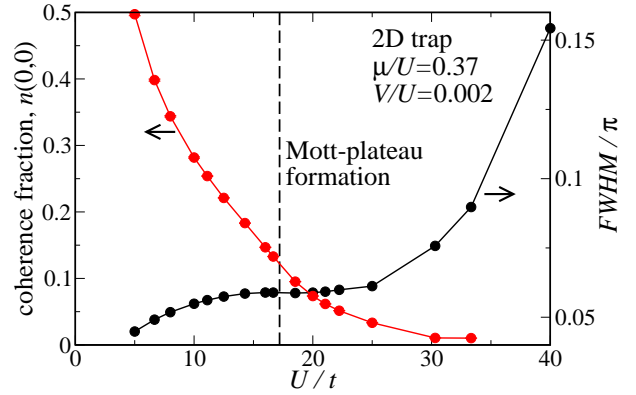


Fig. 4. Evolution of the coherence fraction (the height of the peak, $n(0,0)$) and of the full width at half maximum (FWHM) of the coherence peak as a function of U/t for bosons in a two dimensional parabolic trap with curvature $V/U = 0.002$ and with $\mu/U = 0.37$. The threshold for Mott plateau formation is indicated by the dashed line.

phase transition” between a Mott insulator and a superfluid can be observed by changing e.g. the value of U/t . To study this transition, we calculated the momentum distribution function

$$n(\mathbf{k}) = \frac{1}{N} \sum_{i,j} e^{i(\mathbf{r}_i - \mathbf{r}_j) \cdot \mathbf{k}} \langle b_i^\dagger b_j \rangle, \quad (6)$$

where N is the total number of particles in the system. The momentum distribution in Eq. (6) is normalized, and the coherence fraction is given by the height of the coherence peak, $n(\mathbf{k} = 0)$. Not only is this quantity useful to detect the formation of a Mott plateau as will be shown below: it also is a quantity of interest for experiments, as $n(\mathbf{k})$ can be determined from interference patterns.¹⁴

Fig. 4 displays both the coherence fraction $n(\mathbf{k} = 0)$ and the full width at half maximum (FWHM) of the

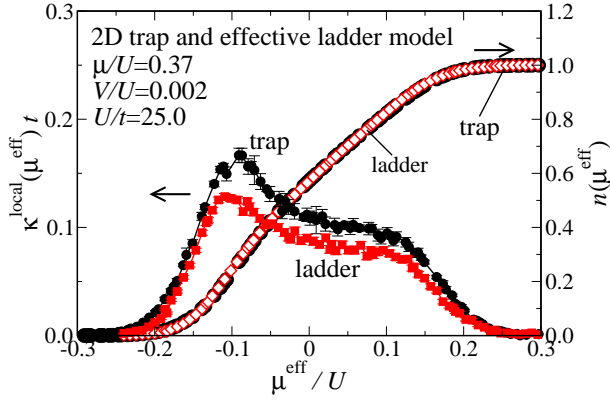


Fig. 5. Local density, n , and local compressibility, κ^{local} , for a two dimensional parabolic trap on a square lattice and for a ladder, as functions of μ^{eff} . The parameters for the trapping potential are $V/U = 0.002$, at $\mu/U = 0.37$, and the parameters of the ladder model are chosen as to cover the whole superfluid region (see Ref. 4).

coherence peak in a two dimensional trap as obtained from the QMC simulations. The ratio U/t at which a Mott plateau forms in the center of the trap is marked by a vertical line. Whereas the coherence fraction does not show any specific feature at the threshold for Mott plateau formation, we observe a change of the curvature in the FWHM at this point. It was shown,⁴ that this appears as a generic feature and that the FWHM can thus serve as an indicator of Mott plateau formation in a confined Bose gas. We also showed that the appearance of fine structure in the momentum distribution (secondary peaks) is not related to the Mott plateau formation, disproving claims in previous work.¹⁴

3.2 Absence of quantum criticality

Fig. 3 suggests that the superfluid region identified by a non vanishing local compressibility is confined to a shell around the central Mott-insulating region. One might then expect that in a two-dimensional trap this shell essentially behaves like a one-dimensional bosonic chain, and displays similar quantum critical behavior. For example, the compressibility of a one-dimensional bosonic chain diverges at the superfluid-insulator transition.¹⁵ However, simulations in a trap indicate no critical features in quantities like the local compressibility.⁴

To further investigate this phenomenon and to simplify simulations, an effective bosonic ladder model was introduced in Ref. 4, that represents the superfluid ring in the original two-dimensional trap. In this model, each leg of the ladder is assigned a different chemical potential, which is chosen such that the first leg is always in a $\langle n \rangle = 0$ Mott insulating phase and the last leg in the $\langle n \rangle = 1$ Mott insulating phase. The chemical potential is then interpolated (for example linearly) between these two values for the other legs of the ladder.

In Fig. 5, we show the local density and the local compressibility κ^{local} as a function of the effective chemical potential μ^{eff} for both simulations, the 2d trap and the ladder model. The overall good agreement of the two sets

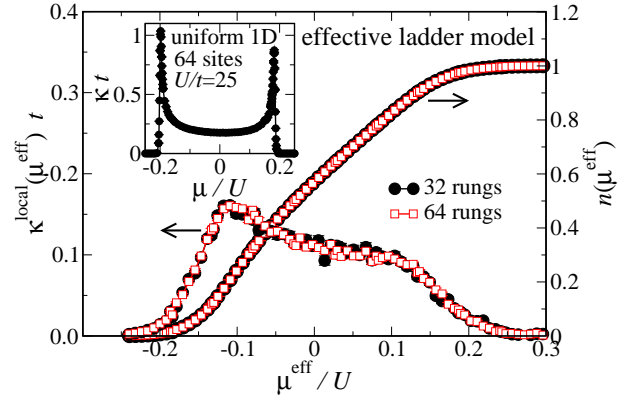


Fig. 6. Local density, n , and local compressibility, κ^{local} , for the Bose-Hubbard model on ladders with different lengths as a function of μ^{eff} . The other parameters of the ladder model are chosen as in Fig. 5. The inset shows the compressibility for the uniform one-dimensional case as a function of μ for a chain with 64 sites, for the same value of U/t as used in the ladder model.

of curves indicates that indeed the ladder model captures the essential physics of the trapped two-dimensional system. The density curves from the trap and the ladder model coincide almost perfectly, indicating the validity of a local density approximation.⁴ There are small differences in the local compressibility between the trap and the ladder system, which are due to the different shape of the local chemical potential in the two systems. Nevertheless, the two different compressibility curves share the same overall shape.

Having shown that the ladder model describes correctly the different physical features found in the trapped system, we can study the occurrence of quantum criticality in this simpler model. In Fig. 6, the local density and the local compressibility of the ladder model are shown for two different system sizes. We observe two very broad peaks in the compressibility, which might indicate quantum critical behavior. However, these peaks do not sharpen upon increasing the length of the ladder, as seen in Fig. 6. The inset of Fig. 6 displays the compressibility of a one-dimensional chain which, in contrast with the ladder results, displays very sharp peaks at the insulating-superfluid phase transition, even for a system of moderate size ($L = 64$).

We thus find that no one-dimensional quantum critical behavior is found in the realistically simulated trapped systems. This is in agreement with the absence of “critical slowing down” observed in the experiments.^{2,3} We thus interpret the “quantum phase transition” seen in the experiments as a crossover of changing fractions of the Mott-insulating and superfluid regions. Critical behavior could however be observed for flat confining potentials. For a more elaborate discussion on the ladder model and the absence of quantum criticality, we refer the reader to Ref. 4.

4. Approaching the Tonks-Girardeau regime

4.1 The Tonks-Girardeau gas

In previous sections, we studied properties of confined ultra-cold bosonic atoms in optical lattices using the Bose-Hubbard Hamiltonian with an on-site repulsion U/t . In the limit of infinite repulsion, $U/t \rightarrow \infty$, this model maps onto a model of hardcore bosons which are constrained to a maximum occupancy of one boson per site. In the continuum limit of the one-dimensional Bose gas, the regime of infinite repulsion defines the Tonks-Girardeau gas,^{16,17} which in many respects behaves similar to fermions due to the enforced impenetrability. The realization of a Tonks-Girardeau gas in trapped bosonic atom systems¹⁸ initially turned out difficult, due to the restricted interaction range accessible from the experimental setup.^{19,20} However, recently Tonks-Girardeau gas behavior was observed in one-dimensional Bose gases in the presence of an optical lattice potential.²¹ The underlying lattice structure increases the effective mass of the bosons, thus increasing the ratio $\gamma = E_{\text{int}}/E_{\text{kin}}$, of interaction energy (E_{int}) to kinetic energy (E_{kin}).²¹ In particular, excellent agreement between the experimental data and calculations based on the fermionization approach to the Tonks-Girardeau gas was obtained in Ref. 21, already for values of $\gamma \approx 5$. In another recent study,²² observation of Tonks-Girardeau gas behavior was reported for similar value of $\gamma \approx 5$ also in the absence of an optical lattice.

4.2 When do we observe Tonks-Girardeau gas behavior?

In the following, we compare both the ground state density distribution and the momentum distribution function of bosons in one-dimensional optical lattices with a harmonic confinement potential to address the question when a system of repulsively interacting bosons shows behavior similar to a Tonks-Girardeau gas. We performed simulations for chains of $N_s = 50$ lattice sites, typical for experimental setup,²¹ and considered different fillings of the system by adjusting the chemical potential.

An appropriate means of quantifying the relevance of the interactions in the presence of an optical lattice is the ratio U/t , given in terms of the microscopic model parameters.²³ To a given value of U/t , an associated effective value of $\gamma_{\text{eff}} = U/(2t\langle n \rangle)$ is obtained by determining the particle density $\langle n \rangle$ during the simulation.²⁴

In Fig. 7 the QMC results for γ_{eff} are shown as a function of U/t for $\mu/t = 0$ and 0.3. For a given value of U/t , the effective value of the interactions, γ_{eff} , is larger for $\mu/t = 0$ than for $\mu/t = 0.3$, due to a lower bosonic density in the first case. We thus expect the behavior of softcore bosons to fit well to that of a Tonks-Girardeau gas for smaller values of U/t for $\mu/t = 0$ than for $\mu/t = 0.3$.

In Fig. 8 (a,b) the spatial density distribution, $n(x)$, and the momentum distribution function, $n(k)$, are shown in the low-density regime for $\mu/t = 0$, with no Mott-insulating region present in the trap. We find that for $U/t = 50$ both quantities are already close to the hardcore limit. Data taken at $U/t = 100$ (not shown) did not exhibit any visible difference to the hardcore limit in this regime. In contrast, for $U = 5$ the density in the trap

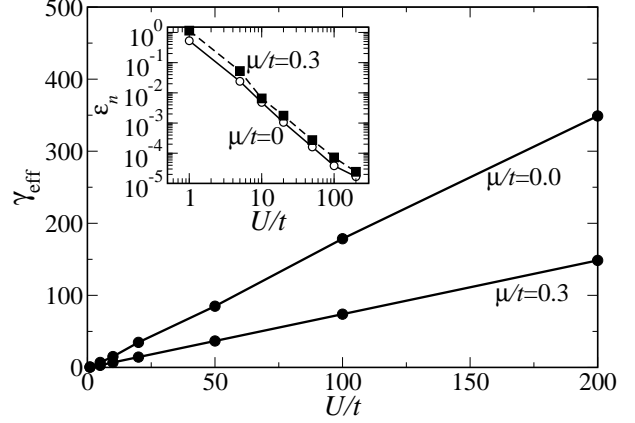


Fig. 7. Effective interaction strength γ_{eff} as a function of the ratio U/t for bosons on one-dimensional optical lattices, inside a harmonic confinement potential of strength $V/t = 10^{-3}$. Results of quantum Monte Carlo simulations are shown for different values of the chemical potential, $\mu/t = 0$, and 0.3. The inset shows the average deviation ϵ_n in the local density between the softcore and hardcore cases as a function of the interaction strength U/t for $\mu/t = 0$ and 0.3.

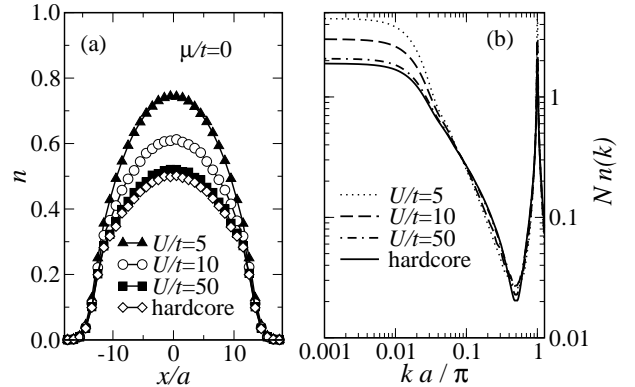


Fig. 8. Density distribution, $n(x)$, and momentum distribution function, $n(k)$, in the ground state of softcore bosons on one-dimensional optical lattices for different values of $U/t = 5, 10, 50$, and for hardcore bosons ($U/t = \infty$), inside a harmonic confinement potential of strength $V/t = 10^{-3}$ and for $\mu/t = 0$.

center is significantly larger than in the hardcore case, as is the coherent fraction $n(k = 0)$. One might thus conclude, as in Ref. 25, that large values of $\gamma > 100$ are needed before the behavior of softcore bosons fits well to that of a Tonks-Girardeau gas. Observing that near the boundary of the system, the density distributions is close in all cases and that due to the low density of bosons in this regime, the value of U is irrelevant, we prefer a different look at this problem.

For a more detailed analysis, we plot the averaged squared deviation $\epsilon_n(U) = 1/N_s \sum_i (n_i(U) - n_i(U = \infty))^2$ as a function of U/t in the inset of Fig. 7. We find, that $\epsilon_n(U)$ decreases algebraically upon increasing U , i.e. $\epsilon_n(U) \propto U^{-\alpha}$, with $\alpha \approx 2$. This shows that the crossover of softcore bosons into the hardcore limit is smooth, and

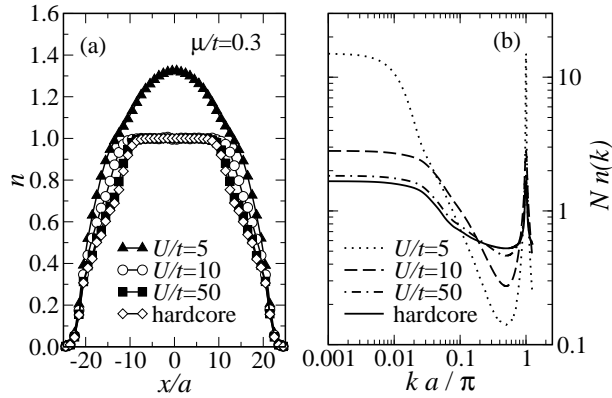


Fig. 9. Density distribution, $n(x)$, and momentum distribution function, $n(k)$, in the ground state of softcore bosons on one-dimensional optical lattices for different values of $U/t = 5, 10, 50$, and for hardcore bosons ($U/t = \infty$), inside a harmonic confinement potential of strength $V/t = 10^{-3}$ and for $\mu/t = 0.3$.

that no finite critical value for U/t exists.

Considering the momentum distribution function $n(k)$ shown in Fig. 8 (b), we find that they are similar to the hardcore limit for all values of U/t in this intermediate-density regime. The main differences occur for the plateau value near $k = 0$, whereas the characteristic slopes of the curves around $k/a \approx \pi/2$ ²¹ are insensitive to the value of U/t . Due to this similar structure, and since the overall scale of $n(k)$ is not fixed by the experimental data, the measured momentum profiles could be fitted in Ref. 21 to the momentum profile of hardcore bosons already for moderate values of γ . Experimentally it is thus difficult to distinguish the softcore regime from the hardcore limit in the low-density region, and behavior similar to a Tonks-Girardeau gas emerges already for moderate values of $\gamma > 5$, as observed in Ref. 21.

Next, we consider the case of an increased bosonic density inside the trap, obtained by increasing the chemical potential. In particular, we consider $\mu/t = 0.3$, and show results for the local density and momentum distribution function in Fig. 9. As seen from Fig. 9 (a), hardcore bosons develop an extended Mott plateau in the trap center for this value of μ . Plateau formation is observed for softcore bosons only for values of $U/t > 10$. Furthermore, the algebraic decrease in $\epsilon_n(U)$ upon increasing U found for $\mu/t = 0$ is also observed for $\mu/t = 0.3$ and with the same exponent of $\alpha \approx 2$. Turning to the momentum distribution functions, we find from Fig. 9 (b), that the momentum profile for $U/t = 5$ and 10 now show significant quantitative differences to the one in the hardcore limit. In particular, the characteristic slopes of the curves near $k/a \approx \pi/2$ now differ significantly from the hardcore case. For high bosonic densities, the differences between softcore and hardcore behavior are thus more pronounced, and easier detectable by measuring the experimentally accessible momentum profile.

5. Conclusion

The main new results of the present paper concern the crossover of softcore bosons into the Tonks-Girardeau

regime. From our simulations we conclude that this crossover appears smooth, and that no finite critical value of the interaction strength U/t exists. Instead, upon increasing U/t , differences in the local density distributions between the softcore and hardcore case decrease algebraically, with an exponent that is insensitive to the density inside the trap.

In the low-density region, the shape momentum profiles of softcore bosons are qualitatively very similar to those observed in the Tonks-Girardeau gas already for moderate values of U/t . This explains the observation in Ref. 21, where the measured momentum profiles could well be fitted using a fermionization approach to the Tonks-Girardeau gas for $\gamma > 5$. The value of γ or U/t beyond which an experiment is well described by a Tonks-Girardeau gas picture depends sensitively on the quantity being measured, the measurement error and the density of bosons. In particular in the low-density region, we find the momentum profile to be rather insensitive to the value of U/t , allowing a description of the softcore boson system in terms of a Tonks-Girardeau gas already at small values of γ . For larger densities, the additional confinement of the superfluid in the hardcore limit leads to quantitative differences in the momentum profile between softcore and hardcore bosons and thus larger values of U/t are needed in order to observe the behavior of a Tonks-Girardeau gas.

Acknowledgments

The numerical calculations were performed using the SSE application package with generalized directed loop techniques⁸ and the worm code application package of the ALPS project,¹⁰ and carried out on the Asgard and Hreidar Beowulf clusters at ETH Zürich.

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